

Zitterbewegung of electronic wave packets in semiconductor nanostructures

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We study the zitterbewegung of electronic wave packets in III-V zinc-blende semiconductor quantum wells due to spin-orbit coupling. Our results suggest a direct experimental proof of this fundamental effect, confirming a long-standing theoretical prediction. For electron motion in a harmonic quantum wire, we numerically and analytically find a resonance condition maximizing the zitterbewegung.

The emerging field of spintronics has generated a large deal of interest in the effects of spin-orbit coupling in semiconductor nanostructures and their possible applications [1]. Spin-orbit coupling is a relativistic effect described by the Dirac equation and its nonrelativistic expansion [2]. In semiconductors spin-orbit coupling of itinerant electrons is much stronger than in vacuum. This is due to the interplay of crystal symmetry and the strong electric fields of the atom cores [3]. In fact, the effective models describing the band structure of III-V semiconductors have many similarities to the Dirac equation. However, the fundamental gap between conduction and valence band in a semiconductor is of order an electron volt or less, which is much smaller than the gap between solutions of positive and negative energy of the free Dirac equation. This observation can serve as a general heuristic explanation for the importance of spin-orbit effects in semiconductors [3].

Another prediction of relativistic quantum mechanics is the zitterbewegung of electrons [2], which, however, has not been observed experimentally yet. For free electrons, i.e. in the absence of an external potential, such an oscillatory motion occurs if solutions of both positive and negative energy of the free Dirac equation have a finite weight in a given quantum state. In this letter we investigate the zitterbewegung of electron wave packets under the influence of the enhanced spin-orbit coupling in III-V zinc-blende semiconductor quantum wells. Strong spin-orbit coupling generally requires large gradients of the external potential, as they are provided by the heavy atom cores in such systems.

An important effective contribution to spin-orbit coupling in such systems is the Rashba term which is due to structure-inversion asymmetry of the confining potential and takes the following form [4]

$$\mathcal{H}_R = (\alpha/\hbar) (p_x \sigma^y - p_y \sigma^x), \quad (1)$$

where \vec{p} is the momentum of the electron confined in a two-dimensional geometry, and $\vec{\sigma}$ the vector of Pauli matrices. The Rashba coefficient α is essentially proportional to the potential gradient across the well and therefore tunable by an external gate. Thus, the single-particle Hamiltonian is given by $\mathcal{H} = \vec{p}^2/2m + \mathcal{H}_R$, where

m is the effective band mass. The components of the time-dependent position operator

$$\vec{r}_H(t) = e^{i\mathcal{H}t/\hbar} \vec{r}(0) e^{-i\mathcal{H}t/\hbar} \quad (2)$$

in the Heisenberg picture read explicitly

$$\begin{aligned} x_H(t) = & x(0) + \frac{p_x}{m}t + \frac{p_y}{p^2} \frac{\hbar}{2} \sigma^z \left(1 - \cos \left(\frac{2\alpha p}{\hbar^2} t \right) \right) \\ & + \frac{p_x}{p^3} \frac{\hbar}{2} (p_x \sigma^y - p_y \sigma^x) \left(\frac{2\alpha p}{\hbar^2} t - \sin \left(\frac{2\alpha p}{\hbar^2} t \right) \right) \\ & + \frac{1}{p} \frac{\hbar}{2} \sigma^y \sin \left(\frac{2\alpha p}{\hbar^2} t \right), \end{aligned} \quad (3)$$

$$\begin{aligned} y_H(t) = & y(0) + \frac{p_y}{m}t - \frac{p_x}{p^2} \frac{\hbar}{2} \sigma^z \left(1 - \cos \left(\frac{2\alpha p}{\hbar^2} t \right) \right) \\ & + \frac{p_y}{p^3} \frac{\hbar}{2} (p_x \sigma^y - p_y \sigma^x) \left(\frac{2\alpha p}{\hbar^2} t - \sin \left(\frac{2\alpha p}{\hbar^2} t \right) \right) \\ & - \frac{1}{p} \frac{\hbar}{2} \sigma^x \sin \left(\frac{2\alpha p}{\hbar^2} t \right), \end{aligned} \quad (4)$$

where the operators \vec{p} and $\vec{\sigma}$ on the right hand sides are in the Schrödinger picture and therefore time-independent.

We now proceed by evaluating the above time-dependent position operators within a Gaussian wave packet with initial spin polarization along the z -direction perpendicular to the quantum well,

$$\langle \vec{r} | \psi \rangle = \frac{1}{2\pi} \frac{d}{\sqrt{\pi}} \int d^2k e^{-\frac{1}{2}d^2(\vec{k}-\vec{k}_0)^2} e^{i\vec{k}\vec{r}} \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (5)$$

Clearly we have $\langle \psi | \vec{r} | \psi \rangle = 0$, $\langle \psi | \vec{p} | \psi \rangle = \hbar \vec{k}_0$, and the variances of the position and momentum operators are $(\Delta x)^2 = (\Delta y)^2 = d^2/2$, $(\Delta p_x)^2 = (\Delta p_y)^2 = \hbar^2/2d^2$. Thus, the group velocity of the wave packet is given by $\hbar \vec{k}_0/m$, while its spatial width is described by the parameter d with the minimum uncertainty product typical for Gaussian wave packets, $\Delta p_x \Delta x = \Delta p_y \Delta y = \hbar/2$.

A direct calculation gives

$$\begin{aligned} \langle \psi | x_H(t) | \psi \rangle = & \frac{\hbar k_{0x}}{m} + \frac{d}{2\pi} e^{-d^2 k_0^2} \int_0^{2\pi} d\varphi \sin \varphi \\ & \cdot \int_0^\infty dq e^{-q^2 + 2dq(k_{0x} \cos \varphi + k_{0y} \sin \varphi)} \\ & \cdot \left(1 - \cos \left(\frac{2\alpha q}{\hbar d} t \right) \right). \end{aligned} \quad (6)$$

In the above expression, φ is a usual polar angle in the xy -plane, and q is a dimensionless integration variable. The time dependence in the integral can be viewed as a zitterbewegung the electron performs under the influence of spin-orbit coupling. Clearly, this integral contribution vanishes for $k_{0y} = 0$, i.e. if the group velocity is along the x -direction. More generally, one finds that

$$\langle \psi | \vec{k}_0 \cdot \vec{r}_H(t) / k_0 | \psi \rangle = \hbar k_0 t / m, \quad (7)$$

which means that the zitterbewegung is always perpendicular to the group velocity of the wave packet. Let us therefore concentrate on the case $k_{0x} = 0$. By expanding the exponential containing the trigonometric functions one derives

$$\begin{aligned} \langle \psi | x_H(t) | \psi \rangle &= \frac{1}{2k_{0y}} \left(1 - e^{-d^2 k_{0y}^2} \right) \\ &- \frac{1}{2k_{0y}} \sum_{n=0}^{\infty} \left[\frac{(dk_{0y})^{2(n+1)}}{n!(n+1)!} \right. \\ &\quad \left. \cdot \int_0^{\infty} dq q^{2n+1} e^{-q^2} \cos\left(\frac{2\alpha q}{\hbar d} t\right) \right]. \quad (8) \end{aligned}$$

Thus, the amplitude of the zitterbewegung is proportional to the wave length of the electron motion perpendicular to it, and the oscillatory zitterbewegung changes its sign if the translational motion is reversed. If the product dk_{0y} is not too large, $dk_{0y} \lesssim 1$, only low values of the summation index n lead to substantial contributions, and the Gaussian factor in the integrand suppresses contributions from large values of q . Thus, a typical scale of this integration variable is leading to sizable contributions is $q \approx 1/\sqrt{2}$. Thus, a typical time scale in the integrand is $T = \sqrt{2}\pi\hbar d/\alpha$, and when averaging the zitterbewegung over times scales significantly larger than T , the cosine term drops giving

$$\overline{\langle \psi | x_H(t) | \psi \rangle} = (1/2k_{0y}) (1 - \exp(-d^2 k_{0y}^2)), \quad (9)$$

i.e. the time-averaged guiding center of the wave packet is shifted perpendicular to its direction of motion. Note that the zitterbewegung is absent for $k_{0y} = 0$ [5].

In the opposite case $dk_{0y} \gg 1$ the Gaussian approaches a δ -function. In this limit one finds (for $k_{0x} = 0$)

$$\langle \psi | x_H(t) | \psi \rangle = (1/2k_{0y}) (1 - \cos(2\alpha k_{0y} t / \hbar)). \quad (10)$$

Here the frequency of the zitterbewegung is $\Omega = 2\alpha k_{0y} / \hbar$, and the guiding center of the wave packet is also shifted in the direction perpendicular to its group velocity. Note that $\hbar\Omega$ is the excitation energy between the two branches of the Rashba Hamiltonian \mathcal{H} at a given momentum $\vec{k} = k_{0y} \vec{e}_y$.

The zitterbewegung of an electron in a quantum well as described above is naturally accompanied by a broadening of the wave packet, where the dominant contribution stems from the dispersive effective-mass term

in the Hamiltonian. Such a broadening might pose an obstacle for experimentally detecting the zitterbewegung. However, the broadening can be efficiently suppressed and limited if the electron moves along a quantum wire. In fact, the motion of electrons in quantum wells is generally under better control if additional lateral confinement is present. We therefore consider a harmonic quantum wire along the y -direction described by $\mathcal{H} = \vec{p}^2/2m + m\omega^2 x^2/2 + \mathcal{H}_R$, where the frequency ω parametrizes the confining potential perpendicular to the wire [6,7]. For this case exact analytical progress as above does not seem to be possible, and we therefore follow a numerical approach combined with an approximate analytical study. To be specific, we consider an electron with a given momentum k_{0y} along the wire and injected initially into the lowest subband of the confining potential with the spin pointing upwards along the z -direction, i.e. the initial wave function for the x -direction is a Gaussian whose width is determined by the characteristic length $\lambda = \sqrt{\hbar/m\omega}$ of the harmonic confinement. In our numerical simulations of the exact time evolution we find again a zitterbewegung perpendicular to the electron motion along the wire with the width of the wave function across the wire being limited by the confining potential. Moreover, the amplitude of the zitterbewegung becomes maximal if the resonance condition $|\hbar\Omega| = |2\alpha k_{0y}| = \hbar\omega$ is fulfilled. This general finding is illustrated in Fig. 1 where the wave number along the wire is fixed to be $k_{0y}\lambda = 5$ and the Rashba parameter α is varied around the resonance condition. Equivalent observation are made if the Rashba coupling is fixed while the wave number k_{0y} is varied. In Fig. 2 we have plotted the amplitude of the zitterbewegung as a function of $\Omega/\omega = 2\alpha k_{0y}/\hbar\omega$ for different values of the wave number k_{0y} along the wire. In this range of parameters, the resonance becomes narrower with increasing k_{0y} , while its maximum value is rather independent of this quantity and remarkably well described by $\lambda/\sqrt{2}$.

A qualitative explanation for this resonance can be given by writing the Hamiltonian in the form $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$ with $\mathcal{H}_0 = \hbar\omega(a^+ a + 1/2) + \hbar^2 k_{0y}^2 / 2m + \alpha k_{0y} \sigma^x$, $\mathcal{H}_1 = -i\sqrt{\hbar m \omega / 2} (\alpha / \hbar) (a - a^+) \sigma^y$, and a, a^+ being the usual harmonic climbing operators [7]. The zitterbewegung is induced by the perturbation \mathcal{H}_1 which can act most efficiently if the unperturbed energy levels of \mathcal{H}_0 are degenerate having opposite spins. This is the case at $|2\alpha k_{0y}| = \hbar\omega$.

Another way to understand this resonance condition is to consider a truncated model where the Hamiltonian has been projected onto the lowest to orbital subbands, an approximation which is known to give very reasonable results for the low-lying energy spectrum of the wire [7]. For a given wave number k_{0y} the truncated Hilbert space is spanned by the states $|0, \uparrow\rangle, |0, \downarrow\rangle, |1, \uparrow\rangle, |1, \downarrow\rangle$, where the arrows denote the spin state with respect to the z -

direction, and 0 and 1 stand for the ground state and the first excited state of the harmonic potential, respectively. When applying the transformation

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix} \quad (11)$$

the projected Hamiltonian and in turn the time evolution operator become block-diagonal,

$$U e^{-\frac{i}{\hbar} H t} U^\dagger = \begin{pmatrix} h_+(t) & 0 \\ 0 & h_-(t) \end{pmatrix} \quad (12)$$

where

$$h_\pm(t) = \left(\mathbf{1} \cos\left(\frac{1}{\hbar} \mu_\pm t\right) - i \frac{\vec{\mu}_\pm}{\mu_\pm} \cdot \vec{\sigma} \sin\left(\frac{1}{\hbar} \mu_\pm t\right) \right) \cdot \exp\left(\frac{i}{\hbar} \left(\hbar \omega + \frac{\hbar^2 k_{0y}^2}{2m} \right) t\right) \quad (13)$$

and $\vec{\mu}_\pm = (\pm \alpha \sqrt{m\omega/2\hbar}, 0, -\hbar\omega/2 \mp \alpha k_{0y})$. Now using

$$U x U^\dagger = \frac{\lambda}{\sqrt{2}} \begin{pmatrix} 0 & \sigma^x \\ \sigma^x & 0 \end{pmatrix} \quad (14)$$

one obtains for the initial state $|0, \uparrow\rangle$ the following time-dependent expectation value

$$\langle 0, \uparrow | x_H(t) | 0, \uparrow \rangle = \frac{\lambda}{\sqrt{2}} \frac{\mu_+^x \mu_-^z + \mu_-^x \mu_+^z}{\mu_+ \mu_-} \cdot \sin(\mu_+ t / \hbar) \sin(\mu_- t / \hbar). \quad (15)$$

At resonance, $\hbar\omega = \pm 2\alpha k_{0y}$, we have $\mu_\mp^z = 0$, and if μ_\pm^x can be neglected compared to μ_\pm^z (which is the case for large enough k_{0y}) the amplitude of the zitterbewegung is approximately $\lambda/\sqrt{2}$, in accordance with the numerics.

We note that the above resonance condition can be reached by tuning either the Rashba coupling or the wave vector of the electron injected into the wire. For instance, for a wire of width $\lambda = 50\text{nm}$ and the band mass of InAs being 0.023 in units of the bare electron mass, one has $\hbar\omega \approx 1\text{meV}$. Typical values for the Rashba parameter α in InAs are of order 10^{-11}eVm [8–14] leading to a wave length $\lambda_{0y} = 2\pi/k_{0y} \approx 100\text{nm}$ at resonance. For GaAs, the band mass is larger while the Rashba coefficient is typically an order of magnitude smaller than in InAs [15], giving a wave length of a few ten nm at resonance for $\lambda = 50\text{nm}$.

We propose that electron zitterbewegung in semiconductor nanostructures as described above can be experimentally observed using high-resolution scanning-probe microscopy imaging techniques as developed and discussed in Refs. [16,17]. As a possible setup, a tip sufficiently smaller than the width of the wire can be moved along the wire and centered in its middle. For an appropriate biasing of the tip, the electron density at its

location is depleted leading to a reduced conductance of the wire. Since the amplitude of the zitterbewegung reflects the electron density in the center of the wire, the zitterbewegung will induce beatings in the wire conductance as a function of the tip position. These beatings are most pronounced at the resonance, see Fig. 1. Note that the oscillations shown there as a function of time can be easily converted to the real-space y -coordinate by multiplying the abscissa by $\hbar k_{0y}/m$. Generally we expect spin-orbit effects in STM experiments to be more pronounced in the presence of additional confinement such as in a quantum wire.

Moreover let us consider spin-orbit coupling of the Dresselhaus type [18–20],

$$\mathcal{H}_D = (\beta/\hbar) (p_y \sigma^y - p_x \sigma^x), \quad (16)$$

which is due to the bulk-inversion asymmetry in zincblende semiconductors, and the coefficient β is determined by the well width along with a material constant [19,20]. Here the components of the time-dependent position operator of an electron in a quantum well read

$$x_H(t) = x(0) + \frac{p_x}{m} t - \frac{p_y}{p^2} \frac{\hbar}{2} \sigma^z \left(1 - \cos\left(\frac{2\beta p}{\hbar^2} t\right) \right) + \frac{p_x}{p^3} \frac{\hbar}{2} (p_y \sigma^y - p_x \sigma^x) \left(\frac{2\beta p}{\hbar^2} t - \sin\left(\frac{2\beta p}{\hbar^2} t\right) \right) - \frac{1}{p} \frac{\hbar}{2} \sigma^x \sin\left(\frac{2\beta p}{\hbar^2} t\right), \quad (17)$$

$$y_H(t) = y(0) + \frac{p_y}{m} t + \frac{p_x}{p^2} \frac{\hbar}{2} \sigma^z \left(1 - \cos\left(\frac{2\beta p}{\hbar^2} t\right) \right) + \frac{p_y}{p^3} \frac{\hbar}{2} (p_y \sigma^y - p_x \sigma^x) \left(\frac{2\beta p}{\hbar^2} t - \sin\left(\frac{2\beta p}{\hbar^2} t\right) \right) + \frac{1}{p} \frac{\hbar}{2} \sigma^y \sin\left(\frac{2\beta p}{\hbar^2} t\right). \quad (18)$$

In much the same way as above, these expressions lead to a zitterbewegung of electronic wave packets in a direction perpendicular to their group velocity. If both Rashba and the Dresselhaus spin-orbit coupling are present, the directional dependence of the zitterbewegung is more complicated, which can be understood terms of the anisotropic dispersion relations arising in this case [21]. The corresponding expressions are rather lengthy and shall not be detailed here. However, in the case where the Rashba coefficient is tuned to be equal in magnitude to the Dresselhaus term, $\alpha = \pm\beta$, the zitterbewegung is absent. This is due to the additional conserved quantity which arises at this point and cancels the many effects of spin-orbit coupling [22,21].

Finally we mention that similar expressions can be derived for the case of heavy holes in the p-type valence band of III-V semiconductors (as opposed to s-type electrons studied so far) being subject to spin-orbit coupling due to structure-inversion asymmetry [23,24]. Again, the

zitterbewegung of a wave packet with its spin pointing initially in the z -direction is perpendicular to the group velocity.

In conclusion, we have studied zitterbewegung of electronic wave packets in III-V zinc-blende semiconductor quantum wells in the presence of spin-orbit coupling of the Rashba and Dresselhaus type. Our results suggest the possibility of a direct experimental proof of this oscillatory motion due to relativistic effects, confirming a long-standing theoretical prediction. Similar results can be derived for the case of heavy holes in quantum wells under the influence of Rashba spin-orbit coupling. A very promising route for such experiments are high-resolution imaging techniques developed recently [16,17]. If the spin of the electron is initially aligned along the z -direction, the zitterbewegung is always perpendicular to the group velocity of the wave packet. For possible experiments quantum wires are particularly attractive. For this case we find a resonance condition maximizing the zitterbewegung. This resonance can be reached by either tuning the Rashba coupling or the electron velocity along the wire.

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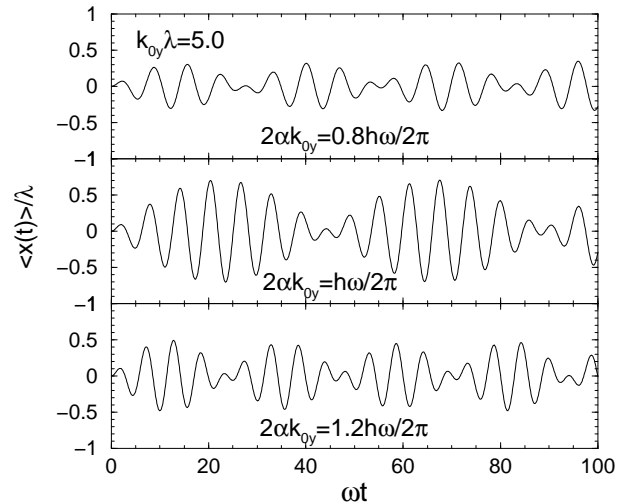


FIG. 1. Zitterbewegung of an electron in a harmonic quantum wire perpendicular to the wire direction. The wave number k_{0y} for the motion along the wire is $k_{0y}\lambda = 5$. The amplitude of the zitterbewegung is maximal at the resonance $2\alpha k_{0y} = \hbar\omega$ (middle panel).

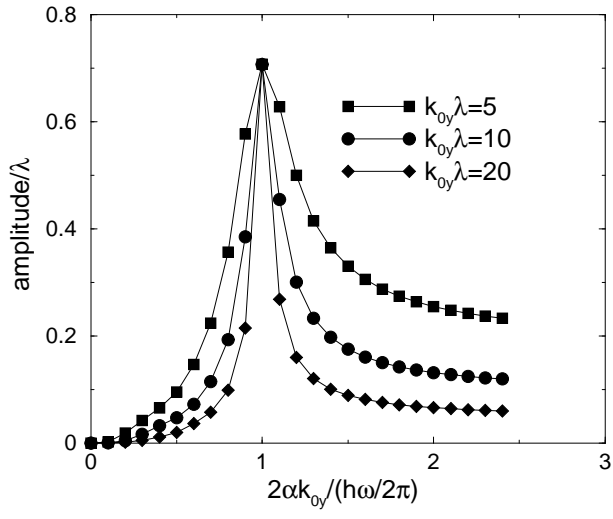


FIG. 2. Amplitude of the zitterbewegung perpendicular to the wire direction as a function of $\Omega/\omega = 2\alpha k_{0y}/\hbar\omega$ for different values of the wave number k_{0y} along the wire.